WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 07:43 pm BST

PDB ID	:	5K50
Title	:	Three-dimensional structure of L-threonine 3-dehydrogenase from Trypanosoma brucei bound to NAD+ and L-allo-threonine refined to 2.23 angstroms
Authors	:	Adjogatse, E.A.; Erskine, P.T.; Cooper, J.B.
Deposited on	:	2016-05-22
Resolution	:	2.26 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

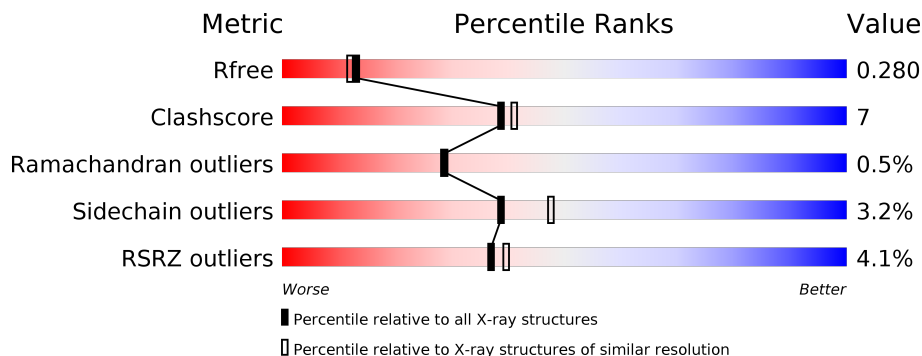|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.280
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		3.2%
RSRZ outliers		4.1%

Worse　　　　　　　　　　　　　　　　　Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	5% / 80% / 19%
1	C	319	3% / 85% / 12% ••
1	E	319	3% / 85% / 14% •
1	G	319	4% / 88% / 12% •
1	I	319	4% / 87% / 12% •
1	J	319	6% / 81% / 18% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

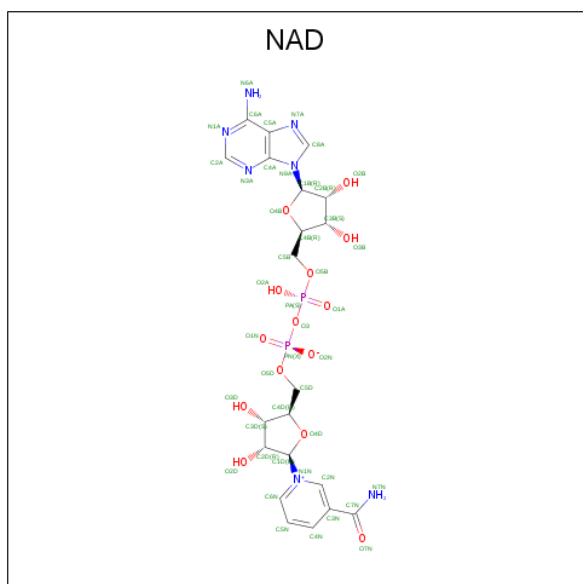| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	J	1402	-	-	X	-
4	ACT	A	1403	-	-	X	-
4	ACT	C	1403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15781 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

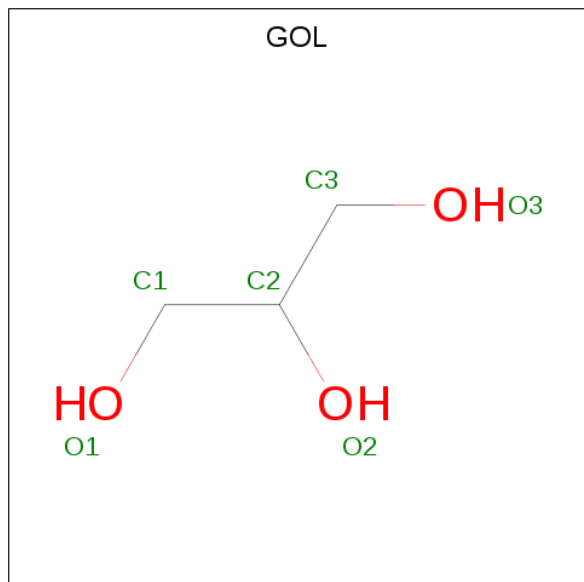- Molecule 1 is a protein called L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total 2493	C 1590	N 415	O 470	S 18	0	0	0
1	C	319	Total 2493	C 1590	N 415	O 470	S 18	0	0	0
1	E	319	Total 2493	C 1590	N 415	O 470	S 18	0	0	0
1	G	319	Total 2532	C 1614	N 422	O 478	S 18	0	7	0
1	I	319	Total 2493	C 1590	N 415	O 470	S 18	0	0	0
1	J	319	Total 2493	C 1590	N 415	O 470	S 18	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total 6	C 3	O 3		0	0
3	J	1	Total 6	C 3	O 3		0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
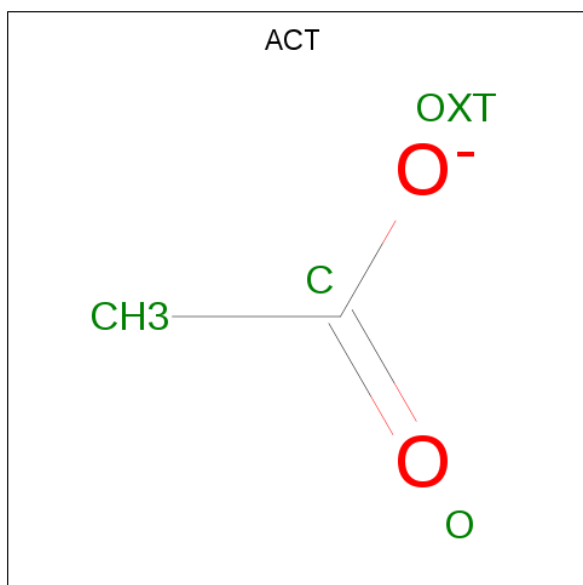
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2		0	0
4	C	1	Total 4	C 2	O 2		0	0
4	C	1	Total 4	C 2	O 2		0	0
4	J	1	Total 4	C 2	O 2		0	0

- Molecule 5 is ALLO-THREONINE (three-letter code: ALO) (formula: $C_4H_9NO_3$).
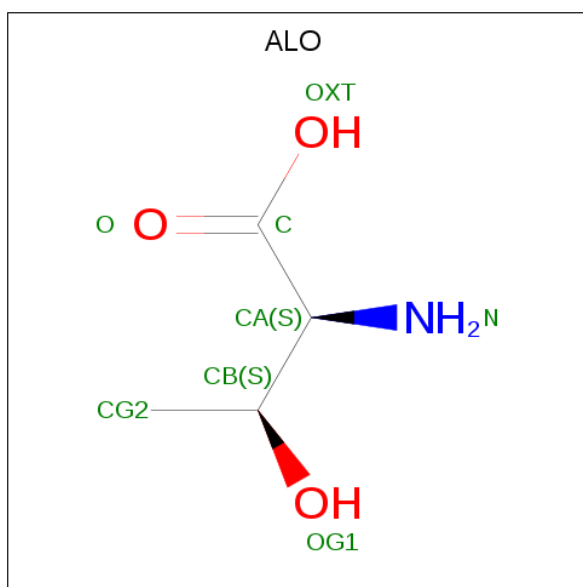
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 8	C 4	N 1	O 3	0	0
5	G	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total 60	O 60	0	0
6	C	65	Total 65	O 65	0	0
6	E	82	Total 82	O 82	0	0
6	G	79	Total 79	O 79	0	0
6	I	79	Total 79	O 79	0	0
6	J	75	Total 75	O 75	0	0

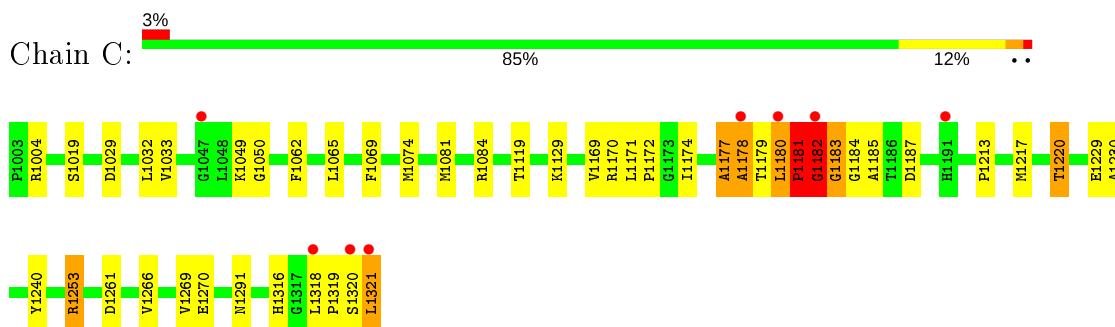# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
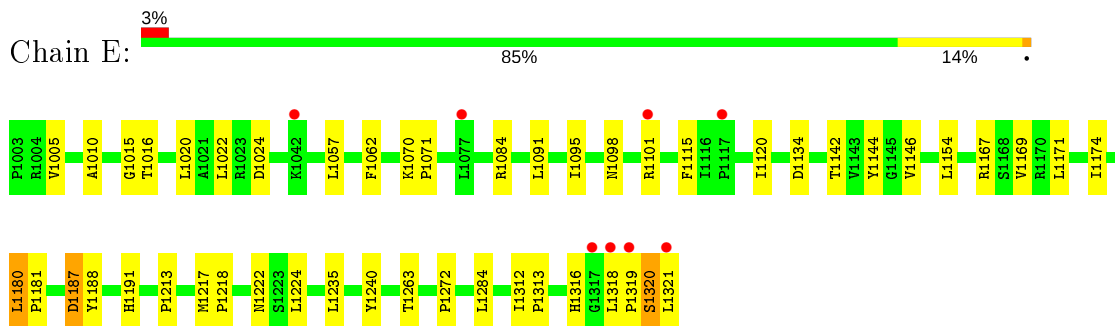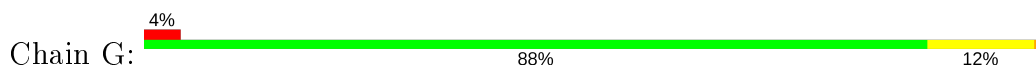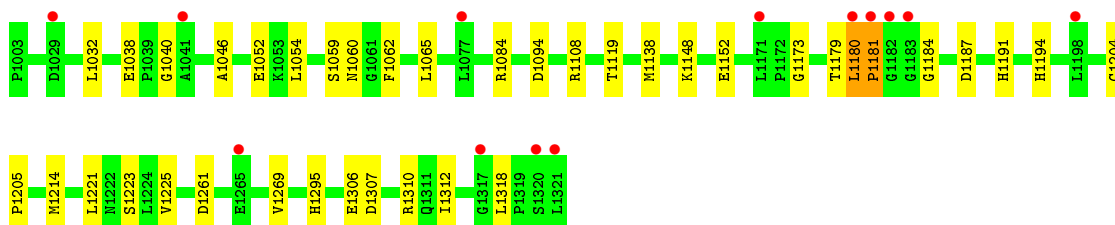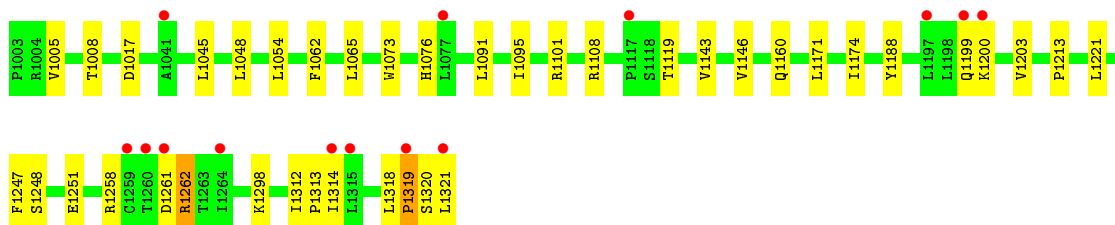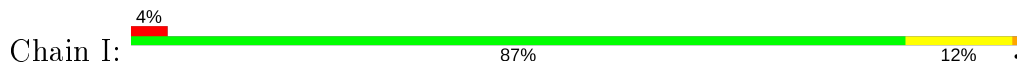
- Molecule 1: L-threonine 3-dehydrogenase
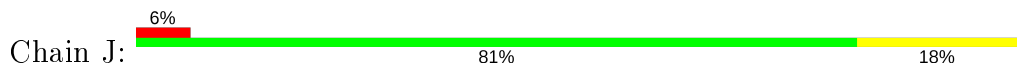

- Molecule 1: L-threonine 3-dehydrogenase

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P1003 D1029 L1032 E1038 P1039 G1040 A1041 A1046 E1052 K1053 L1054 S1059 N1060 G1061 F1062 L1065 L1077 R1084 D1094 R1108 T1119 M1138 K1148 E1152 L1171 P1172 G1173 T1179 L1180 P1181 G1182 G1183 G1184 D1187 H1191 H1194 L1198 C1204

P1205 M1214 L1221 N1222 S1223 L1224 V1225 D1261 E1265 V1269 H1295 E1306 D1307 R1310 Q1311 I1312 G1317 Q1318 P1319 S1320 L1321

● Molecule 1: L-threonine 3-dehydrogenase

Chain I:

4%

87% 12%

P1003 R1004 V1005 T1008 D1017 A1041 L1045 L1048 L1054 F1062 L1065 W1073 H1076 L1077 L1091 I1095 R1101 R1108 P1117 S1118 T1119 V1143 V1146 Q1160 L1171 I1174 Y1188 L1197 L1198 Q1199 K1200 V1203 P1213 L1221

F1247 S1248 E1251 R1258 C1259 T1260 D1261 R1262 T1263 I1264 K1298 I1312 P1313 I1314 L1315 L1318 P1319 S1320 L1321

● Molecule 1: L-threonine 3-dehydrogenase

Chain J:

6%

81% 18%

P1003 R1004 Q1013 I1014 L1018 S1019 L1020 D1024 A1028 D1029 L1032 V1033 S1034 D1035 V1036 G1040 A1041 K1042 L1045 A1046 G1047 L1048 K1049 F1062 L1065 F1069 I1080 M1081 R1084 E1088 P1089 D1090 L1091 A1092 M1093 D1094 V1097 N1098 D1135 K1148 E1152 P1172

G1173 I1174 P1181 G1182 G1183 G1184 A1185 T1186 D1187 Y1188 A1189 I1190 H1191 L1197 C1204 P1205 V1206 L1207 L1212 L1221 N1222 S1223 R1237 I1242 D1261 R1262 T1263 I1264 E1265 V1269 E1270 Q1274 A1277 D1282 D1286 E1306 D1307 M1308 I1312 P1313 G1317 L1318 L1321

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.03Å 273.06Å 55.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.09 – 2.26 31.09 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.09-2.26) 99.7 (31.09-2.26)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.207 , 0.281 0.214 , 0.280	Depositor DCC
R_{free} test set	4815 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.2	EDS
L-test for twinning[2]	$< |L| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15781	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4958e-04.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, NAD, ALO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.66	1/2549 (0.0%)	0.79	2/3458 (0.1%)
1	C	0.71	1/2549 (0.0%)	0.87	5/3458 (0.1%)
1	E	0.66	0/2549	0.79	0/3458
1	G	0.67	0/2589	0.83	2/3513 (0.1%)
1	I	0.67	0/2549	0.81	1/3458 (0.0%)
1	J	0.61	0/2549	0.82	4/3458 (0.1%)
All	All	0.66	2/15334 (0.0%)	0.82	14/20803 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1181	PRO	N-CD	5.78	1.55	1.47
1	A	1251	GLU	CD-OE2	-5.27	1.19	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1183	GLY	N-CA-C	7.40	131.61	113.10
1	J	1237	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	I	1108	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	G	1108	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	J	1237	ARG	NE-CZ-NH2	-6.12	117.24	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1182	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2504	39	0
1	C	2493	0	2504	46	0
1	E	2493	0	2504	36	0
1	G	2532	0	2542	35	0
1	I	2493	0	2504	25	0
1	J	2493	0	2504	46	0
2	A	44	0	26	3	0
2	C	44	0	26	1	0
2	E	44	0	26	1	0
2	G	44	0	26	0	0
2	I	44	0	26	1	0
2	J	44	0	26	1	0
3	A	6	0	8	1	0
3	E	12	0	16	2	0
3	G	6	0	8	0	0
3	I	12	0	16	1	0
3	J	12	0	16	4	0
4	A	4	0	3	7	0
4	C	8	0	6	2	0
4	J	4	0	3	0	0
5	C	8	0	8	3	0
5	G	8	0	8	0	0
6	A	60	0	0	2	0
6	C	65	0	0	2	0
6	E	82	0	0	3	0
6	G	79	0	0	2	0
6	I	79	0	0	2	0
6	J	75	0	0	2	0
All	All	15781	0	15310	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 229 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1180[B]:LEU:HD12	1:G:1181[B]:PRO:CD	1.12	1.56
1:G:1180[B]:LEU:CD1	1:G:1181[B]:PRO:HD3	1.00	1.48
1:J:1080:ILE:HD11	1:J:1091:LEU:HG	1.25	1.15
1:J:1181:PRO:HB2	1:J:1191:HIS:ND1	1.63	1.14
1:J:1080:ILE:CD1	1:J:1091:LEU:HG	1.78	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/319 (99%)	303 (96%)	14 (4%)	0	100	100
1	C	317/319 (99%)	294 (93%)	17 (5%)	6 (2%)	8	4
1	E	317/319 (99%)	303 (96%)	14 (4%)	0	100	100
1	G	324/319 (102%)	299 (92%)	21 (6%)	4 (1%)	13	9
1	I	317/319 (99%)	297 (94%)	19 (6%)	1 (0%)	41	46
1	J	317/319 (99%)	303 (96%)	14 (4%)	0	100	100
All	All	1909/1914 (100%)	1799 (94%)	99 (5%)	11 (1%)	29	25

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1180	LEU
1	G	1180[A]	LEU
1	G	1180[B]	LEU

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Mol	Chain	Res	Type
1	C	1183	GLY
1	C	1178	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/276 (100%)	266 (96%)	10 (4%)	35	42
1	C	276/276 (100%)	267 (97%)	9 (3%)	38	46
1	E	276/276 (100%)	268 (97%)	8 (3%)	42	51
1	G	279/276 (101%)	270 (97%)	9 (3%)	39	47
1	I	276/276 (100%)	268 (97%)	8 (3%)	42	51
1	J	276/276 (100%)	267 (97%)	9 (3%)	38	46
All	All	1659/1656 (100%)	1606 (97%)	53 (3%)	39	47

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1187	ASP
1	G	1060	ASN
1	J	1090	ASP
1	E	1235	LEU
1	E	1320	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1191	HIS
1	G	1060	ASN
1	J	1191	HIS
1	E	1060	ASN
1	J	1060	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	E	1402	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	A	1402	-	5,5,5	0.52	0	5,5,5	1.27	1 (20%)
5	ALO	C	1402	-	4,7,7	1.23	0	4,9,9	1.56	2 (50%)
3	GOL	I	1403	-	5,5,5	0.38	0	5,5,5	0.80	0
3	GOL	J	1403	-	5,5,5	0.40	0	5,5,5	0.40	0
5	ALO	G	1403	-	4,7,7	0.50	0	4,9,9	0.14	0
3	GOL	J	1402	-	5,5,5	0.24	0	5,5,5	0.77	0
3	GOL	G	1402	-	5,5,5	0.61	0	5,5,5	0.61	0
2	NAD	J	1401	-	42,48,48	1.61	6 (14%)	50,73,73	1.58	8 (16%)
4	ACT	A	1403	-	1,3,3	0.44	0	0,3,3	0.00	-
3	GOL	I	1402	-	5,5,5	0.53	0	5,5,5	0.83	0
4	ACT	C	1403	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
2	NAD	I	1401	-	42,48,48	1.53	5 (11%)	50,73,73	1.26	6 (12%)
2	NAD	G	1401	-	42,48,48	1.56	8 (19%)	50,73,73	1.26	5 (10%)
2	NAD	E	1401	-	42,48,48	2.16	6 (14%)	50,73,73	1.35	5 (10%)
3	GOL	E	1403	-	5,5,5	0.51	0	5,5,5	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAD	C	1401	-	42,48,48	1.66	7 (16%)	50,73,73	1.52	8 (16%)
2	NAD	A	1401	-	42,48,48	1.48	4 (9%)	50,73,73	1.54	8 (16%)
4	ACT	J	1404	-	1,3,3	0.41	0	0,3,3	0.00	-
4	ACT	C	1404	-	1,3,3	0.17	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1402	-	-	3/4/4/4	-
5	ALO	C	1402	-	-	4/4/8/8	-
3	GOL	I	1403	-	-	2/4/4/4	-
3	GOL	J	1403	-	-	0/4/4/4	-
3	GOL	J	1402	-	-	2/4/4/4	-
3	GOL	G	1402	-	-	2/4/4/4	-
2	NAD	J	1401	-	-	4/26/62/62	0/5/5/5
5	ALO	G	1403	-	-	1/4/8/8	-
3	GOL	I	1402	-	-	2/4/4/4	-
3	GOL	E	1403	-	-	0/4/4/4	-
2	NAD	I	1401	-	-	5/26/62/62	0/5/5/5
2	NAD	G	1401	-	-	2/26/62/62	0/5/5/5
2	NAD	E	1401	-	-	3/26/62/62	0/5/5/5
2	NAD	C	1401	-	-	6/26/62/62	0/5/5/5
2	NAD	A	1401	-	-	5/26/62/62	0/5/5/5
3	GOL	E	1402	-	-	4/4/4/4	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1401	NAD	O7N-C7N	8.45	1.40	1.24
2	A	1401	NAD	O7N-C7N	6.20	1.36	1.24
2	I	1401	NAD	O7N-C7N	6.10	1.35	1.24
2	C	1401	NAD	O7N-C7N	5.89	1.35	1.24
2	J	1401	NAD	O7N-C7N	5.76	1.35	1.24

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1401	NAD	O4B-C1B-C2B	-5.93	98.26	106.93
2	C	1401	NAD	N3A-C2A-N1A	-4.97	120.91	128.68
2	E	1401	NAD	N3A-C2A-N1A	-4.47	121.69	128.68
2	A	1401	NAD	N3A-C2A-N1A	-4.47	121.69	128.68
2	C	1401	NAD	C4A-C5A-N7A	-4.17	105.05	109.40

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1402	ALO	N-CA-CB-CG2
5	C	1402	ALO	N-CA-CB-OG1
5	C	1402	ALO	C-CA-CB-CG2
5	C	1402	ALO	C-CA-CB-OG1
3	I	1403	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	GOL	1	0
5	C	1402	ALO	3	0
3	J	1402	GOL	4	0
2	J	1401	NAD	1	0
4	A	1403	ACT	7	0
3	I	1402	GOL	1	0
4	C	1403	ACT	2	0
2	I	1401	NAD	1	0
2	E	1401	NAD	1	0
3	E	1403	GOL	2	0
2	C	1401	NAD	1	0
2	A	1401	NAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
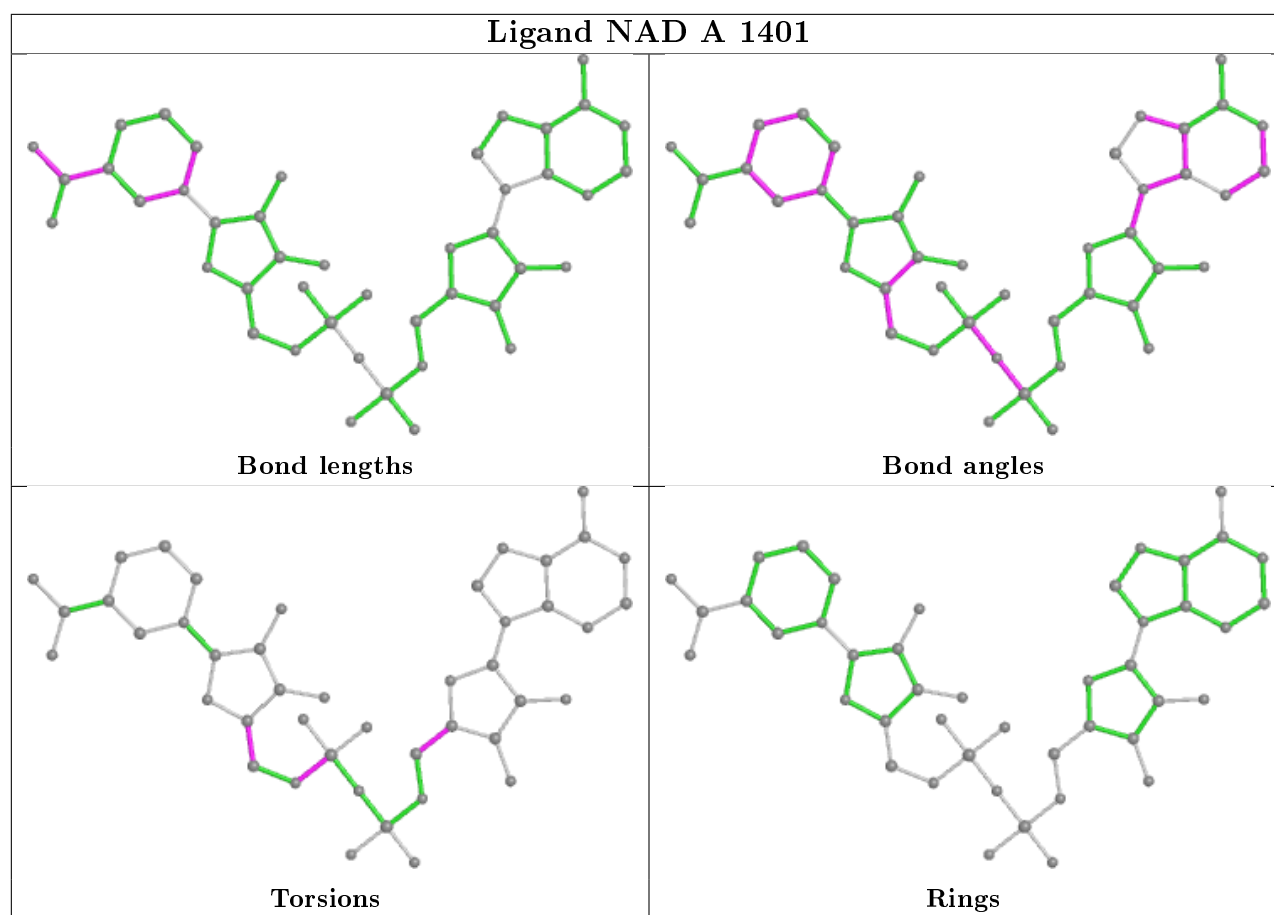
Ligand NAD J 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD I 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD G 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD E 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 1401

Bond lengths

Bond angles

Torsions

Rings
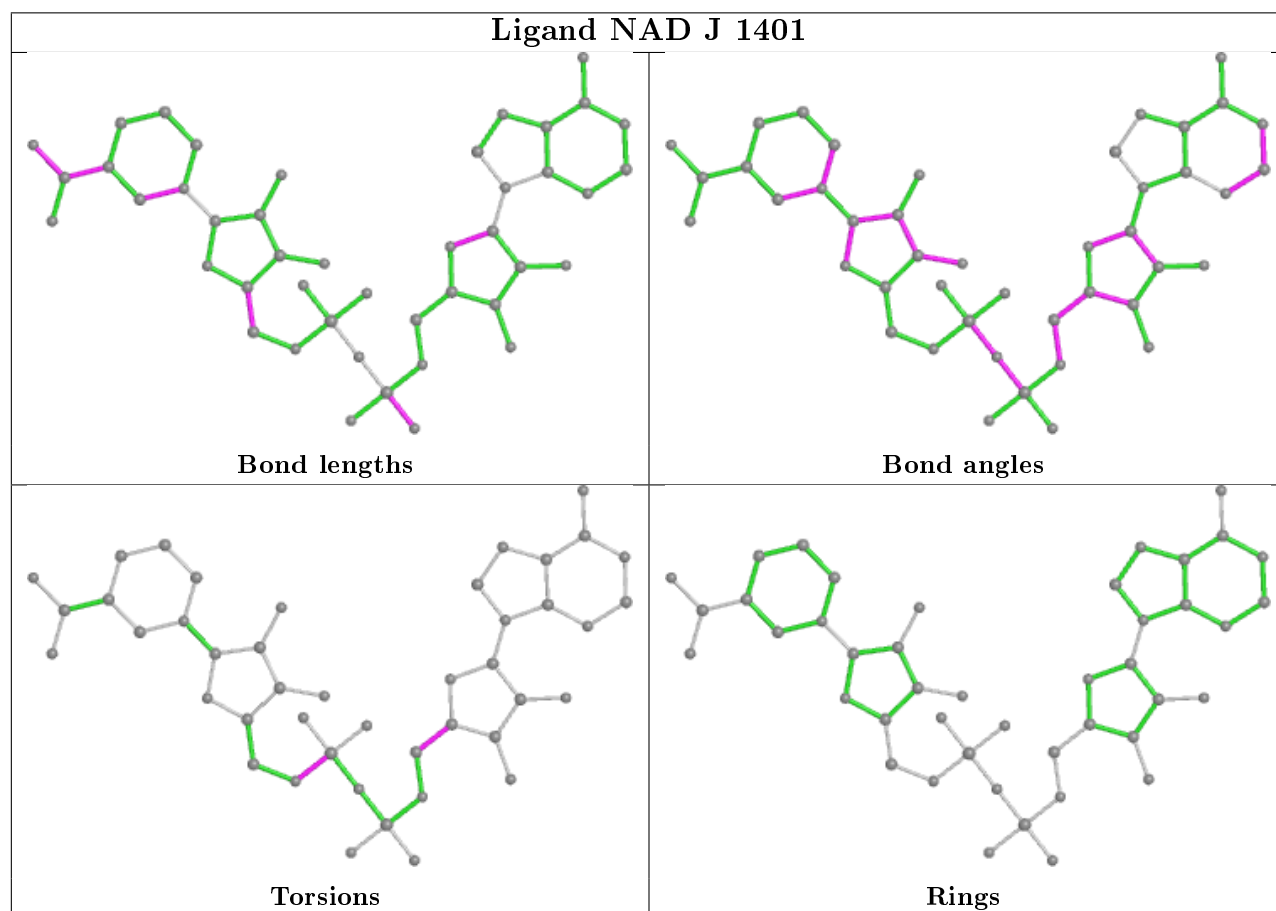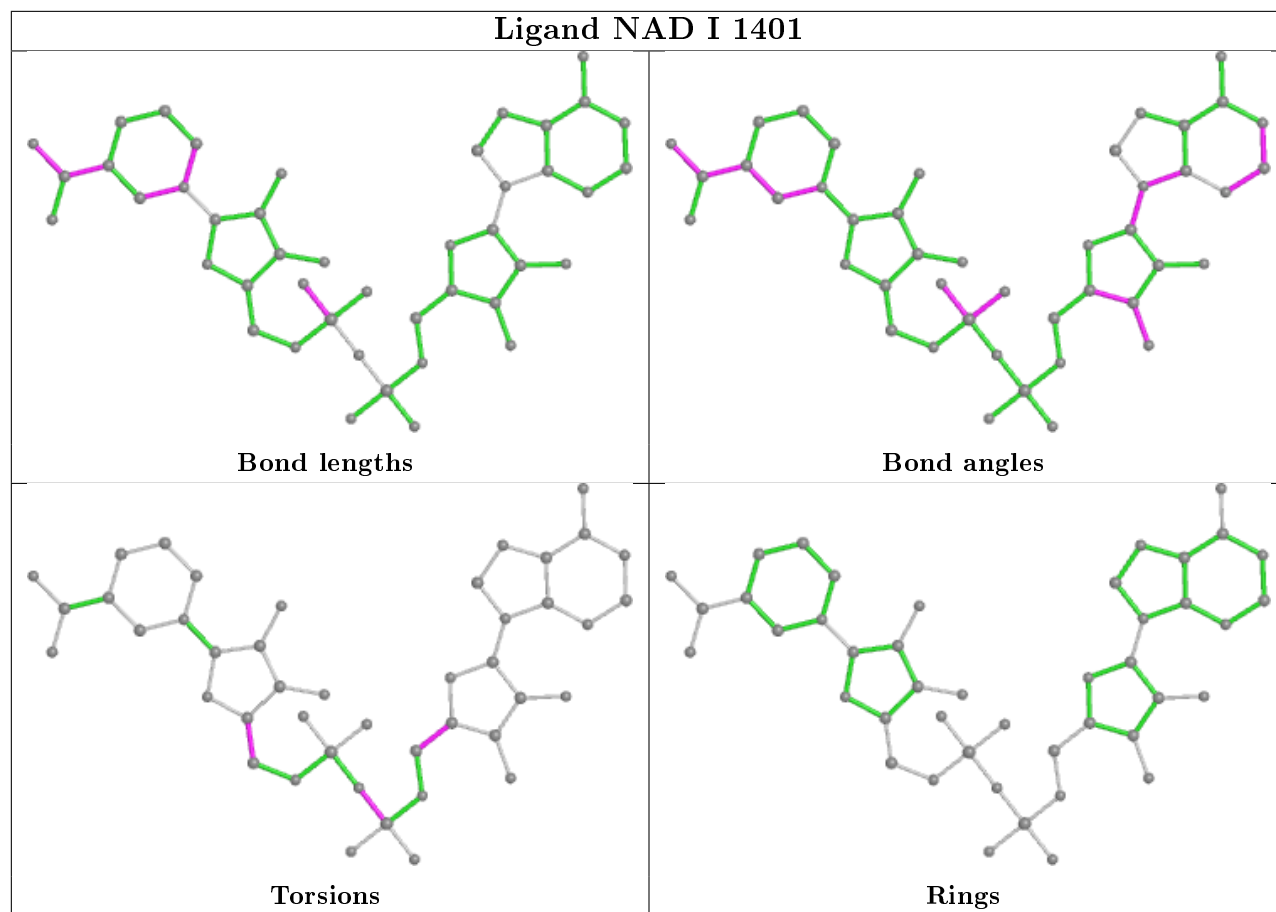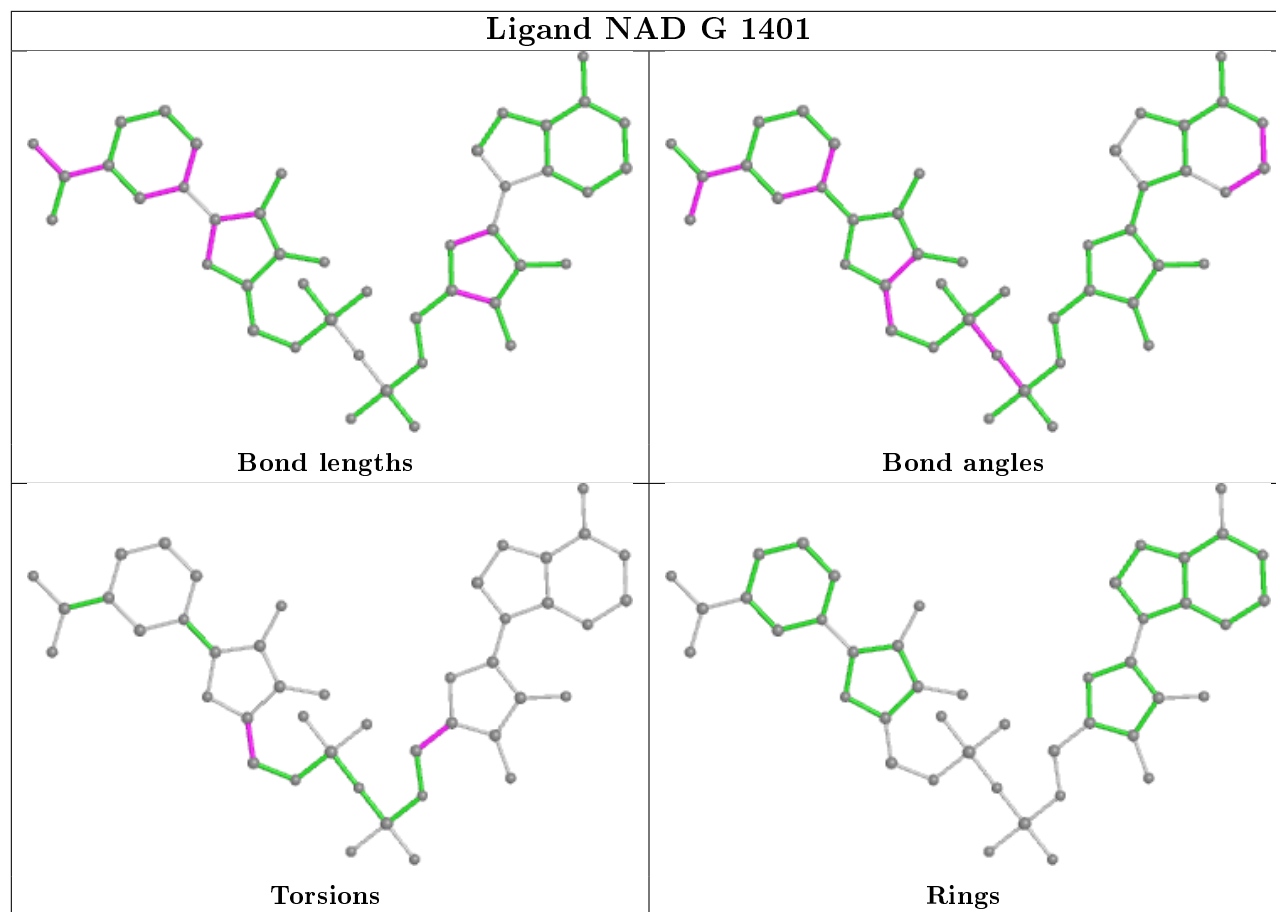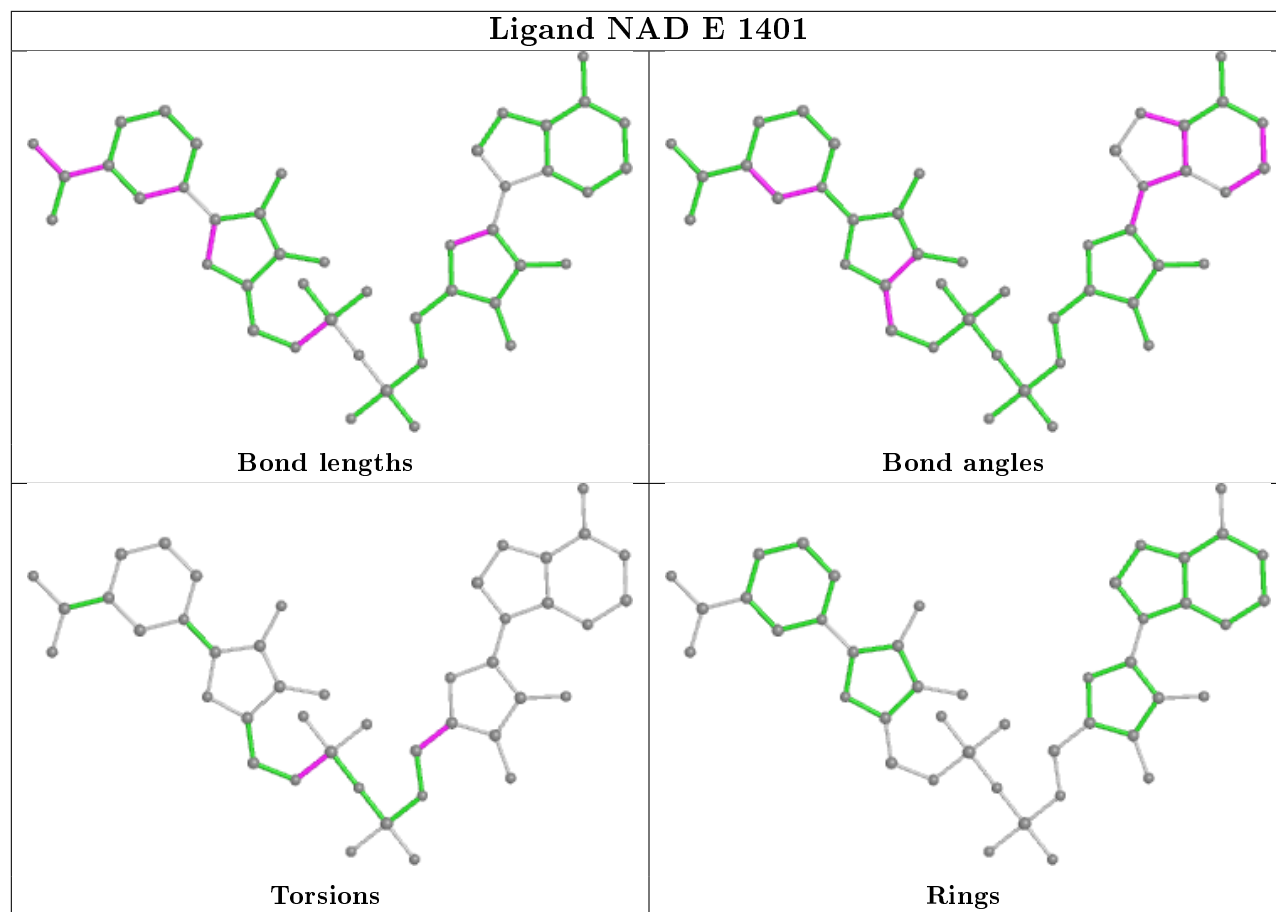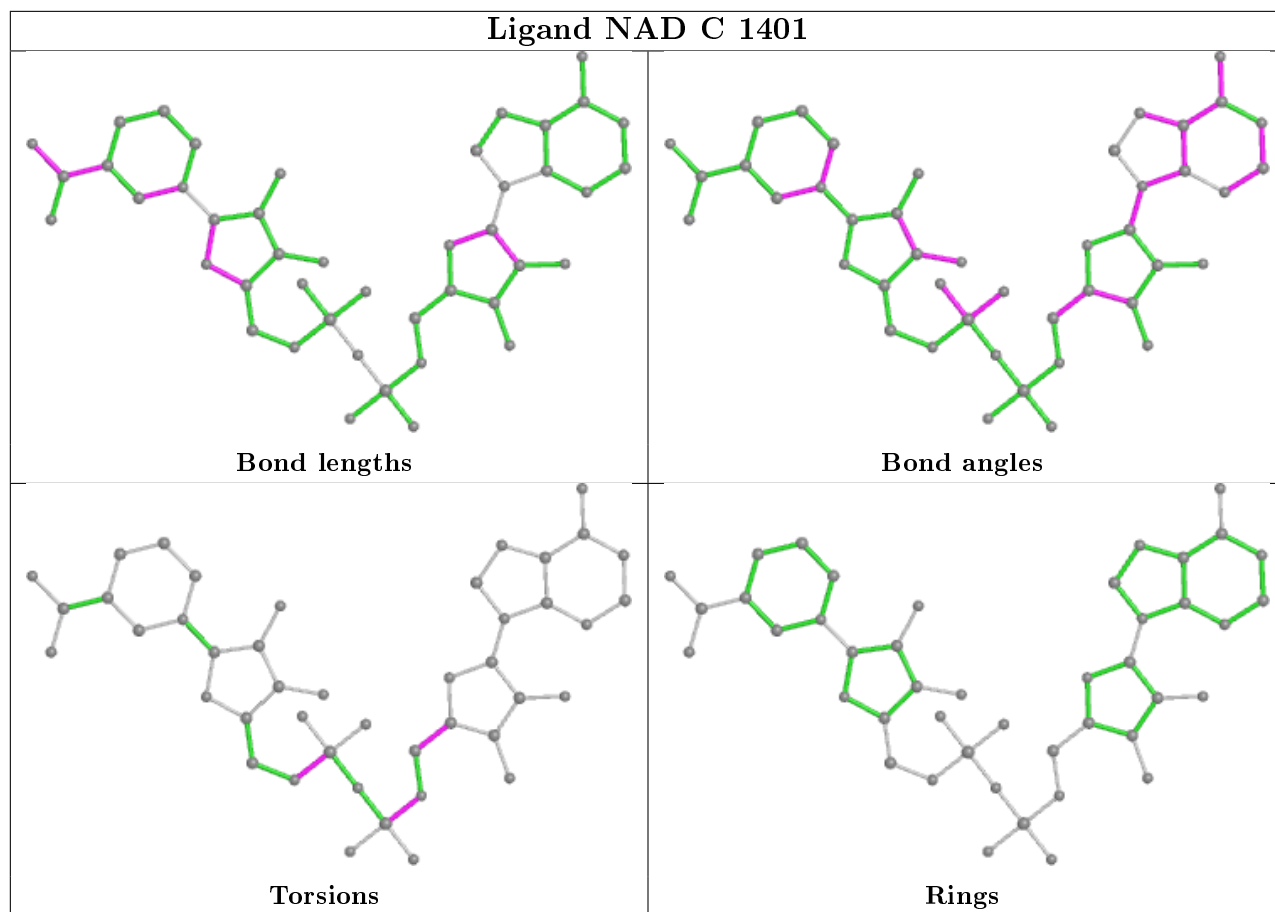
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	319/319 (100%)	0.14	16 (5%)	28	31	18, 34, 61, 91	0
1	C	319/319 (100%)	0.01	8 (2%)	57	60	14, 27, 60, 77	0
1	E	319/319 (100%)	-0.04	8 (2%)	57	60	19, 31, 56, 86	0
1	G	319/319 (100%)	-0.04	13 (4%)	37	40	17, 29, 50, 74	0
1	I	319/319 (100%)	0.07	14 (4%)	34	37	15, 30, 67, 96	0
1	J	319/319 (100%)	0.20	20 (6%)	20	22	16, 33, 63, 83	0
All	All	1914/1914 (100%)	0.06	79 (4%)	37	40	14, 31, 60, 96	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1321	LEU	7.2
1	C	1321	LEU	6.1
1	E	1321	LEU	5.9
1	J	1182	GLY	5.2
1	A	1182	GLY	5.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	J	1402	6/6	0.80	0.25	49,51,52,56	0
3	GOL	G	1402	6/6	0.82	0.27	41,43,45,45	0
5	ALO	C	1402	8/8	0.84	0.22	22,25,29,32	0
5	ALO	G	1403	8/8	0.85	0.20	32,39,41,52	0
3	GOL	I	1403	6/6	0.86	0.15	45,48,48,49	0
4	ACT	C	1403	4/4	0.86	0.20	39,47,49,50	0
4	ACT	A	1403	4/4	0.86	0.19	51,52,56,59	0
4	ACT	C	1404	4/4	0.89	0.23	49,50,52,54	0
3	GOL	J	1403	6/6	0.89	0.14	47,49,51,52	0
3	GOL	E	1403	6/6	0.90	0.20	32,35,36,39	0
3	GOL	E	1402	6/6	0.90	0.13	37,39,40,41	0
3	GOL	A	1402	6/6	0.93	0.23	30,31,35,39	0
3	GOL	I	1402	6/6	0.93	0.17	32,33,36,36	0
2	NAD	G	1401	44/44	0.94	0.14	19,24,27,30	0
2	NAD	J	1401	44/44	0.94	0.15	19,24,27,30	0
2	NAD	A	1401	44/44	0.95	0.14	20,26,30,34	0
2	NAD	I	1401	44/44	0.95	0.12	21,24,27,28	0
4	ACT	J	1404	4/4	0.96	0.34	25,27,28,29	0
2	NAD	E	1401	44/44	0.96	0.12	16,22,25,29	0
2	NAD	C	1401	44/44	0.97	0.13	17,20,23,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD G 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
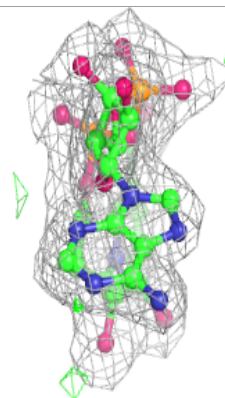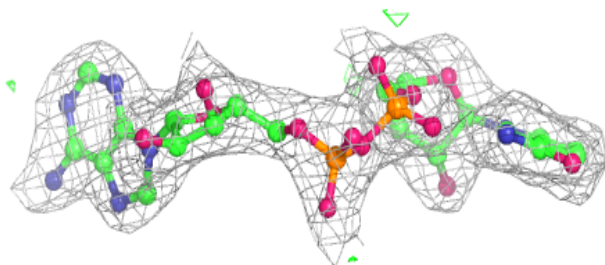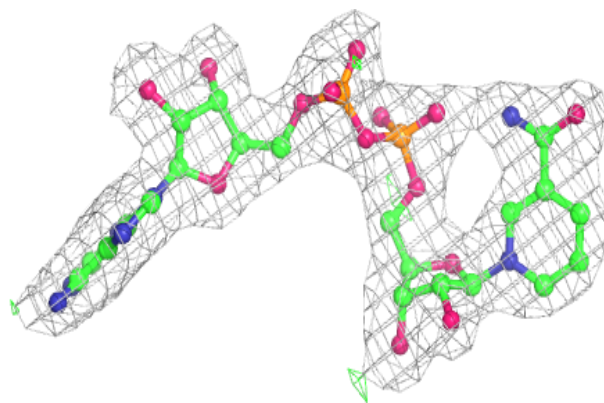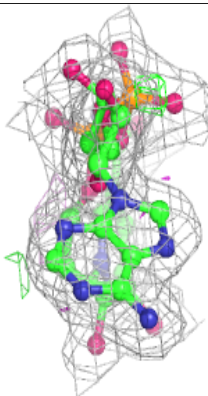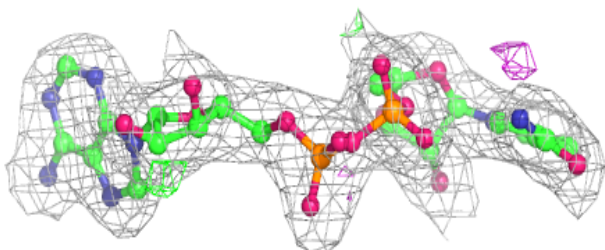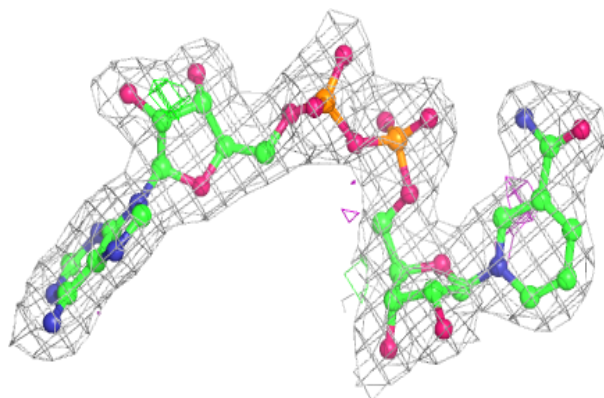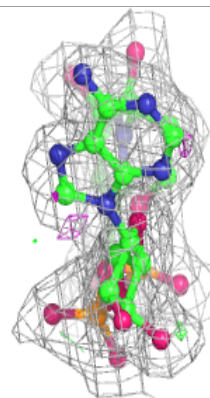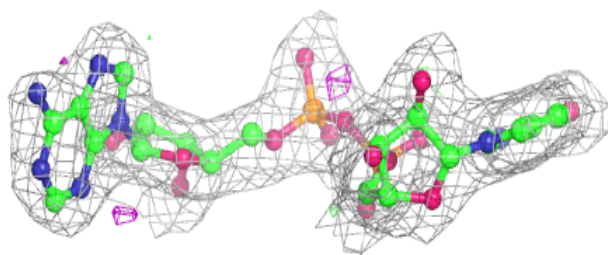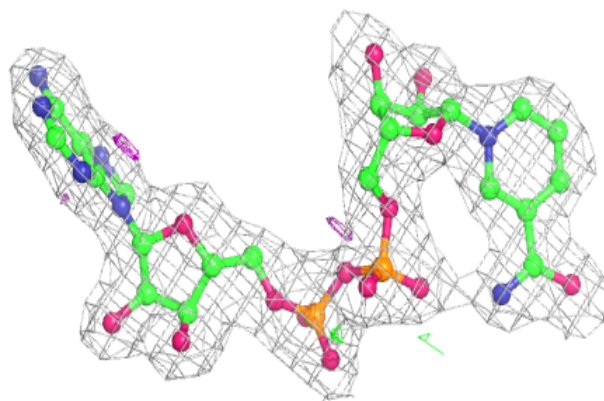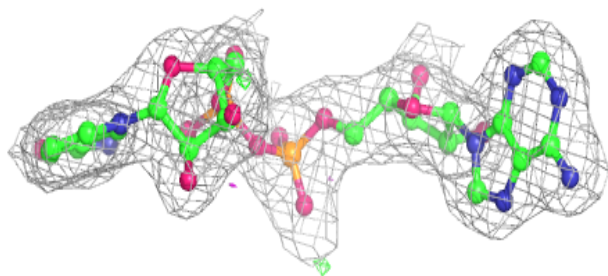mF_o-DF_c (at 3 rmsd) in purple (negative)
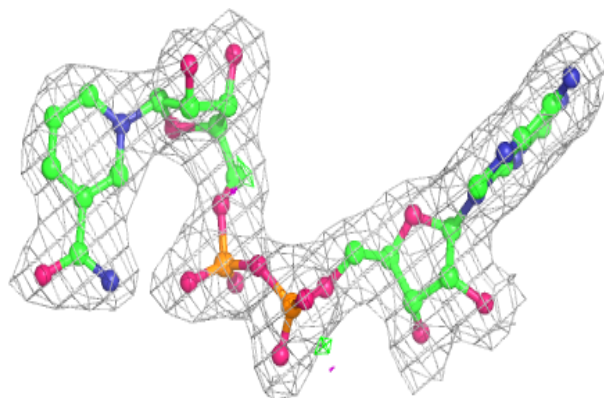and green (positive)
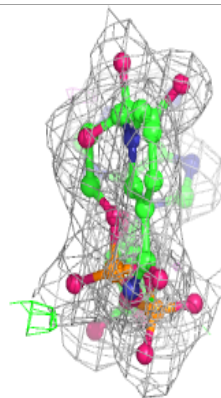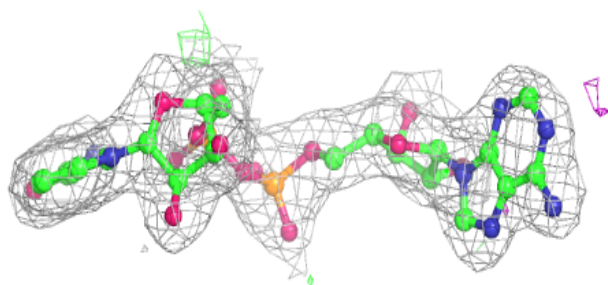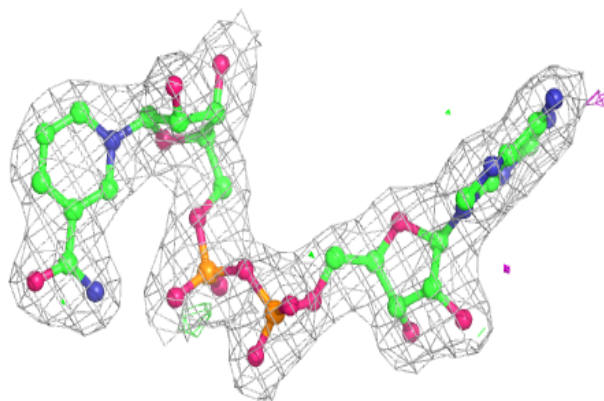
Electron density around NAD J 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
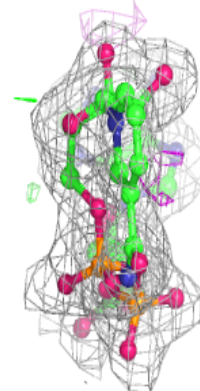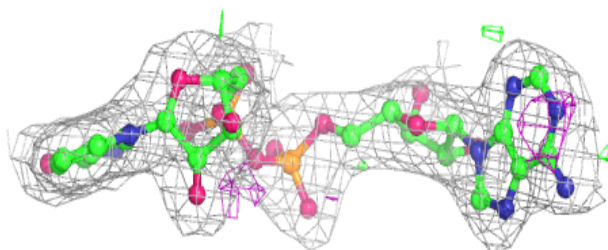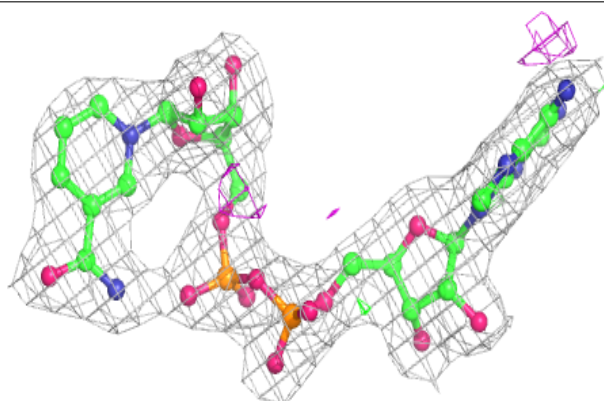
Electron density around NAD A 1401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD I 1401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD E 1401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAD C 1401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.